

Determination of the effect of the medium on the thermodynamic parameters of the conformational transformations of 3-substituted 2,4-dithia-3,5-dihydro-1H-cycloocta[d,e]naphthalenes by double fitting of exchange-broadened PMR spectra

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Abstract

The thermodynamic parameters of the conformational equilibrium for 3-substituted 2,4-dithia-3,5-dihydro-1H-cycloocta[d,e] naphthalenes in various solvents were obtained by the PMR method with temperature variation. The "double fitting" procedure makes it possible to eliminate the systematic error due to the effect of temperature on the spectral parameters of each of the forms. Here the linear temperature dependence of the nonequivalence in the chemical shifts of the AB quadruplets leads to good agreement between the theoretical and experimental line shapes over the whole temperature range of the investigations. The effect of the medium on the enthalpy of the equilibrium can be explained in terms of the reactive field model. © 1991 Plenum Publishing Corporation.

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